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EVALUATION OF NEUTRON INDUCED REACTION CROSS SECTIONS ON GOLD

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ABSTRACT

A new evaluation of neutron induced reactions on the ^{197}Au nucleus in the energy regions below 500 eV and from 4 keV to 100 keV is presented. Complete evaluated data files in ENDF-6 format have been produced by joining the evaluation with corresponding files from the ENDF/B-VII.1 library. The evaluation in the unresolved resonance region between 4 keV and 100 keV is based on a generalized single-level representation compatible with the energy-dependent option of the ENDF-6 format. The average partial cross sections have been expressed in terms of transmission coefficients by applying the Hauser-Feshbach statistical reaction theory including width fluctuations. The transmission coefficients have been obtained from a combined analysis of the capture cross section resulting from the cross section standards evaluation project and theoretical non-fluctuating cross sections derived from a dispersive coupled channel optical model. The evaluated cross sections have been validated by a comparison with transmission and capture data obtained at the time-of-flight facility GELINA. The evaluated files have been processed with the latest updates of NJOY.99 to test their format and application consistency as well as to produce a continuous-energy data library in ACE format for use in Monte Carlo codes. The ACE files have been utilized to study the effect of the evaluated resonance parameters on results of lead slowing-down experiments. The evaluated files will be implemented in the next release of the JEFF-3 library which is maintained by the Nuclear Energy Agency of the OECD.

1. INTRODUCTION

Gold is an important material for nuclear applications. The $^{197}\text{Au}(n,\gamma)$ cross section is recommended as a standard for neutron induced reaction cross section measurements at 0.0253 eV and in the energy region between 200 keV and 2.5 MeV [1-3]. Fitted values of the capture cross section from 2.5 keV up to 200 keV were also derived within the standards cross section project. However, this cross section is not released as a standard [1-3]. The $^{197}\text{Au}(n,\gamma)$ cross section is often used as well as a reference cross section for astrophysical applications in the energy region below 200 keV [4]. Furthermore, neutron induced reactions on Au (e.g. (n,2n) reaction) are proposed as a standard for high energy neutron dosimetry [5] and are considered as a test-case for many nuclear reaction model codes.

Despite the importance of neutron reactions on gold, the energy region in the major general purpose nuclear data libraries [6-10] is only split up in a resolved resonance region (RRR) up to about 5 keV and a continuum region above 5 keV. At present no unresolved resonance region (URR) is considered. Hence, no evaluation of cross sections for neutron induced reactions on Au in terms of average resonance parameters is defined in the major evaluated data libraries. This might cause substantial bias effects on results of calculations of integral quantities when resonance structures together with the Doppler effect play an important role due to self-shielding. The only evaluation of ^{197}Au in terms of average resonance parameters in the URR is found in the TENDL-2011 nuclear data library [11]. Unfortunately, this evaluation has been performed with incorrect values of the elastic degrees of freedom for five of the spin sequences. In addition, the choice to limit the URR upper boundary to the inelastic threshold (77.75 keV) can be considered as an extra constraint.

In this report an ENDF-6 compatible [12] evaluation of cross section data for ^{197}Au in terms of average resonance parameters for neutron energies between 4 keV and 100 keV is described. The evaluation includes covariance information on the resulting parameters. The evaluation for the URR was joined with the corresponding files taken from the ENDF/B-VII.1 nuclear data library [6]. Before joining the files, the RRR part of ENDF/B-VII.1 below 500 eV was revised using results of transmission, capture and self-indication measurements carried out by Massimi et al. [13]. The evaluated files have been processed with the latest updates of NJOY.99 [14] to test the consistency of the files and to study the effect of the evaluated resonance parameters on results of integral experiments.

2. EVALUATION METHODOLOGY

The partial cross sections in the energy region between 4 keV and 100 keV have been expressed in terms of transmission coefficients applying the Hauser-Feshbach statistical reaction theory with width fluctuations. An approach similar to the one applied for ^{232}Th was followed [15,16]. To ensure compatibility with the energy-dependent options of the ENDF-6 SLBW approach [12] a restricted number of approximations are implemented. The contribution of the distant levels is taken into account following the standard description scheme, but with energy dependent distant level parameters and consequently, an energy dependent scattering radius. The independent parameters used to describe the average total and partial cross sections were the following quantities related to zero neutron energy:

- a scattering radius R' independent from the orbital angular momentum ℓ ;
- neutron strength functions $S_{n,\ell=0,1,2}$ for s-, p- and d-waves ($\ell = 0, 1$ and 2); and
- capture transmission coefficients $T_{\gamma,0}^{2^+}$ and $T_{\gamma,0}^{2^-}$ for s- and p-wave, respectively.

The neutron strength functions and scattering radius R' were adjusted to reproduce the absorption and shape elastic cross sections calculated with the dispersive coupled channel optical model (DCCOM) potential RIPL1483 derived by Capote et al. [17]. The DCCOM smooth and weak energy dependence at energies below 100 keV was approximated by second order polynomials. The coupled-channel OPTMAN code [18] incorporated into the EMPIRE system [19] was used for the optical model calculations. The capture transmission coefficients at zero energy were adjusted by fitting to the capture cross section recommended by Carlson et al. [1,2]. This cross section is the result of international cooperative efforts to improve cross section standards by a Subgroup formed by the Working Party on International Evaluation Cooperation of the Nuclear Energy Agency and a Coordinated Research Project Organized by the International Atomic Energy Agency. The evaluation of the $^{197}\text{Au}(n,\gamma)$ cross section in the energy region between 2.5 keV and 2.8 MeV was performed by a simultaneous analysis of various types of experimental data: energy dependent, spectrum-averaged and thermal data, including ratios and absolute results. The analysis was based on the results of 62 experiments using a least-squares adjustment code GMA, developed by Poenitz [20]. The full data set is given in Refs. [1, 2].

The final parameters are reported in Table 1. The resulting total and capture cross section are compared with experimental data in Fig. 1 and Fig.2, respectively. In Fig. 1 the total cross section recommended in ENDF/B-VII.1 is also shown. The total cross section obtained at the time-of-flight facility GELINA [21] results from measurements performed at a 50 m station using a 3 mm thick metal gold disc [22]. The capture data have been derived from capture experiments carried out at a 12.5 m station of GELINA using a 0.5 mm and 1.0 mm thick metal gold disc [23]. The total energy detection principle was applied in combination with the pulse height weighting technique. The data have been normalized to the saturated resonance at 4.9 eV. The total and capture experiments of Ref. [22, 23] were carried out following the recommendations described in Ref. [24]. The results of Ref. [22] and Ref. [23] have not been included in the evaluation of the capture cross section of Ref. [1, 2] and in the derivation of the optical model parameters of Ref. [17]. The good agreement between the calculated and experimental data in Fig. 1 and 2 confirms the predictive power of the DCCOM of Capote et al. [17] for optical model cross sections and the accuracy of the capture cross section of Ref. [1,2]. The results in Fig. 1 also suggest that the total cross section recommended in ENDF/B-VII.1 is primarily based on the work of Seth [25] and Poenitz [26] without considering the data produced by Purtov et al. [27].

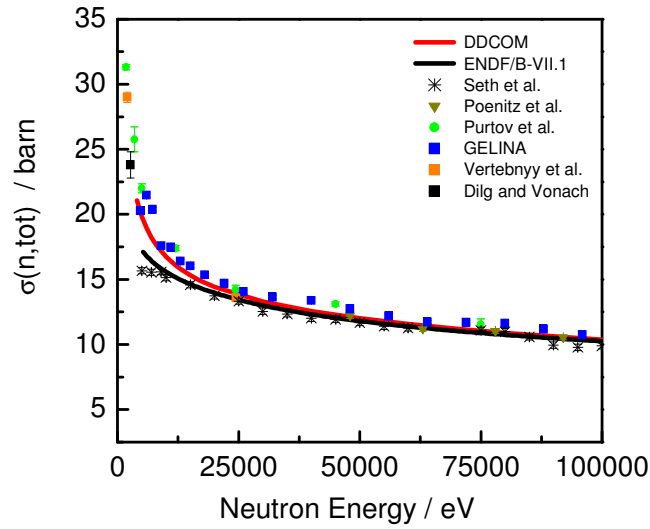


Fig. 1. Comparison of experimental total cross sections with the cross section recommended in ENDF/B-VII.1 and the one derived from the DCCOM of Capote et al. [17]. The experimental data are from Seth [25], Dilg and Vonach [28], Vertebnyi et al. [29], Poenitz et al. [26], Purtov et al. [27] and Sirakov et al. [22].

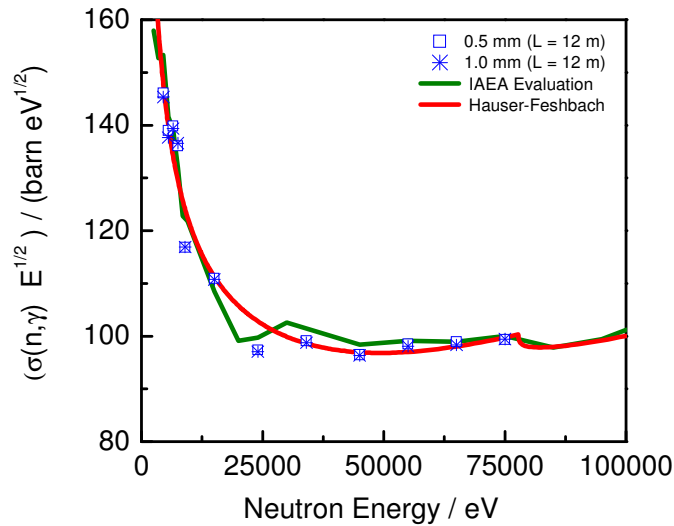


Fig. 2. Comparison of the cross section derived from capture measurements at GELINA [23] with the cross section recommended by the IAEA working group [1,2] and the one resulting from a HF-representation as reported in this work.

Parameter, $\bar{\theta}$		$100 \times \frac{u_{\theta}}{\theta}$	Correlation matrix, $\rho(\bar{\theta}, \bar{\theta}')$					
R'	9.14 fm	1.9	1.000	-0.388	-0.646	-0.583	0.522	0.617
$S_{n,0}$	$1.715 \cdot 10^{-4}$	4.1		1.000	0.786	0.701	-0.796	-0.695
$S_{n,1}$	$5.30 \cdot 10^{-5}$	35			1.000	0.854	-0.875	-0.899
$S_{n,2}$	$3.511 \cdot 10^{-4}$	23				1.000	-0.692	-0.975
$T_{\gamma 0}^{2+}$	$3.471 \cdot 10^{-2}$	5.7					1.000	0.752
$T_{\gamma 0}^{2-}$	$1.018 \cdot 10^{-2}$	28						1.000

Table 1. Average parameters to describe the total and capture cross section of ^{197}Au in the URR. The covariance matrix has been derived by considering the scattering radius as an adjustable parameter without any prior information. The uncertainties in the third column are relative uncertainties in percentage.

The covariance matrix $C_{\bar{\theta}}$ of the average parameters, represented by the parameter vector $\bar{\theta}$, was derived by conventional uncertainty propagation [24]:

$$C_{\bar{\theta}} = (D_{\bar{\theta}}^T C_Z^{-1} D_{\bar{\theta}})^{-1}, \quad (1)$$

where $D_{\bar{\theta}}$ is the design matrix composed of the first partial derivatives of the theoretical cross sections with respect to the parameters. The covariance matrix of the experimental observables is represented by C_Z . This matrix is constructed by assuming a 2% correlated and 1.5% uncorrelated uncertainty for the total cross section and a 1.5% correlated and 1.5% uncorrelated uncertainty for the capture cross section. The final covariance matrix is given in Table 1. These correlated uncertainties are typical uncertainties that can be reached when total and capture cross section measurements are carried out following the recommendations of Ref. [24]. The resulting uncertainties on the calculated total and capture cross sections are shown in Fig. 3 and Fig. 4.

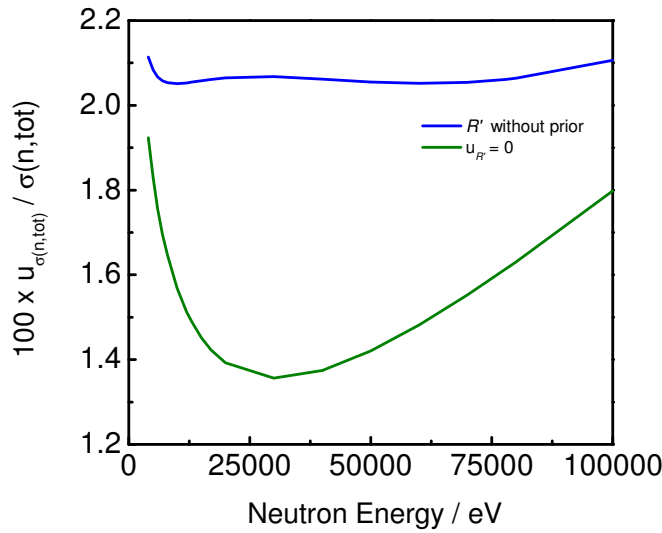


Fig. 3. Relative uncertainty of the total cross section resulting from a Hauser-Feshbach representation described in this work. The results of two uncertainty propagation calculations are shown: one with the scattering radius considered as an adjustable parameter without any prior information and one with a known scattering radius, i.e. a zero uncertainty for the scattering radius $u_{R'} = 0$.

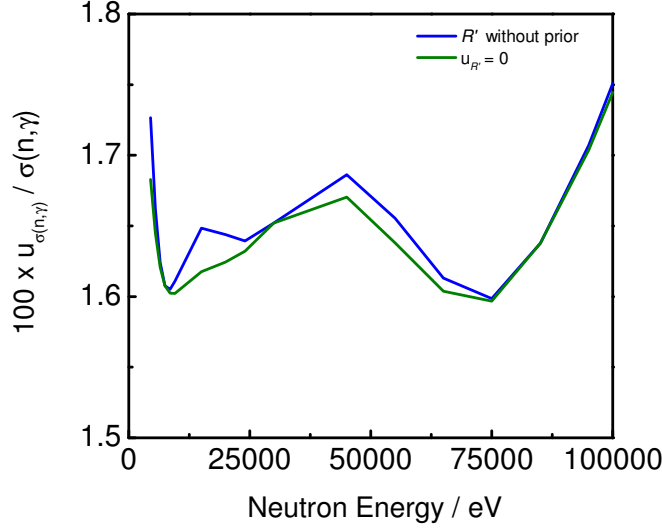


Fig. 4. Relative uncertainty of the capture cross section resulting from a Hauser-Feshbach representation described in this work. The results of two uncertainty propagation calculations are shown: one with the scattering radius considered as an adjustable parameter without any prior information and one with a known scattering radius, i.e. a zero uncertainty for the scattering radius $u_R = 0$.

3. ENDF-6 COMPATIBLE FILES FOR $^{197}\text{Au} + n$

The evaluation for the URR, from 4 keV to 100 keV, was joined with the corresponding files taken from the ENDF/B-VII.1 nuclear data library. Before joining the files the resolved resonance region (RRR) part of the ENDF/B-VII.1 evaluation below 500 eV was revised based on the resonance parameters resulting from transmission and capture cross section data obtained at GELINA [12]. The parameters of the first negative resonance were adjusted to reproduce the thermal capture cross section $\sigma(n_{\text{th}}, \gamma) = 98.67 \pm 0.10$ b and the coherent scattering length $b_c = 7.90 \pm 0.07$ fm recommended by Holden and Holden [30] and Koester et al. [31], respectively. To account for missing levels in the RRR a background contribution from thermal up to 4 keV was introduced in MF/MT=3/102. Based on the evaluation in the URR described in section 2 the missing contribution due to p- and d-waves at 4 keV is about 4.75 % or 115 mb. In the URR from 4 keV to 100 keV a small background contribution was added in MF/MT=3/102 at the expense of MF/MT=3/2 in order to make the evaluated capture cross section identical to the one produced by the standard group Ref. [1,2]. The total, elastic scattering and capture cross section of the present evaluation at thermal energy together with the resonance integrals are summarized in Table 2. The data are for a temperature $T = 0$ and the resonance integrals are derived with a lower limit of 0.5 eV and an upper limit of 100 keV.

	Cross section at 0.0253 eV	RI
	barn	Barn
(n,tot)	106.98	1924.72
(n,n)	8.31	381.30
(n, γ)	98.67	1543.39

Table 2. Total, elastic scattering and capture cross section at thermal energy and the resonance integrals (RI) resulting from the evaluation presented in this work. The data are for a temperature $T = 0$ K and the resonance integrals are derived with a lower limit of 0.5 eV and an upper limit of 100 keV.

Measures were taken to reduce bias effects due to the assumption in the ENDF-6 format (model) about the orbital momentum conservation. This assumption is not consistent with the Hauser-Feshbach (compound nucleus) theory. Bias effects due to this assumption occur in the case of non-even-even nuclei (ground state spin $I \neq 0$), for spin sequences of double orbital momentum contribution, e.g. $J^\pi = 1^+, 2^+$ for $^{197}\text{Au} + n$. For example, at 100 keV the biased ENDF-6 model for the $^{197}\text{Au}(n, \gamma)$ and $^{197}\text{Au}(n, n')$ cross sections results in a 9.6% and 6.2%

increase, respectively, compared to using a rigorous Hauser-Feshbach model with the same parameters. The problem can be solved by adjusting (reducing) the corresponding ENDF d-wave reaction (non-elastic) widths. Since the total cross section remains intact in such a procedure, the elastic one gets also corrected. Even the simplest remedy demonstrated in the file, as a zero iteration to adapt the d-wave reaction widths, diminished the ENDF model bias effect to -3.14 % in capture. The next iteration can be done assuming linearity between the bias in the reaction cross section and the corresponding d-wave reaction widths of $J^\pi = 1^+$ and 2^+ . The results were compared making use of the IRMM URR code, which can process both ways - by sticking to the ENDF-6 model with and without the assumption for l -conservation.

Since the ENDF6-format in the URR does not handle covariances of the scattering radius, the full covariance matrix as given in Table 1 cannot be used. Therefore, the uncertainty propagation was repeated by supposing that the scattering radius is known with an uncertainty $u_{R'} = 0$. The resulting covariance matrix is given in Table 3. The corresponding uncertainties of the total and capture cross section are compared in Fig. 3 and Fig. 4 with the results of the procedure described in section 2. Fig. 3 and Fig. 4 reveal that the uncertainty on the total cross section is underestimated, while the one on the capture cross section is almost not affected. To construct File 32 a very small relative uncertainty on the level spacing was introduced, thus assuring that the relative covariance elements for the reduced neutron widths as well as for the s- and p-wave capture widths can be presented by the relative covariance elements of the neutron strength functions and the corresponding capture transmission coefficients, respectively.

Parameter, $\bar{\theta}$		$100 \times \frac{u_{\theta}}{\theta}$	Correlation matrix, $\rho(\bar{\theta}, \bar{\theta}')$				
R'	9.14 fm	0					
$S_{n,0}$	$1.715 \cdot 10^{-4}$	3.7	1.000	0.761	0.634	-0.754	-0.628
$S_{n,1}$	$5.30 \cdot 10^{-5}$	27		1.000	0.770	-0.826	-0.833
$S_{n,2}$	$3.511 \cdot 10^{-4}$	19			1.000	-0.560	-0.963
$T_{\gamma 0}^{2+}$	$3.471 \cdot 10^{-2}$	4.9				1.000	0.640
$T_{\gamma 0}^{2-}$	$1.018 \cdot 10^{-2}$	22					1.000

Table 3. Average parameters to describe the total and capture cross section of ^{197}Au in the URR. The covariance matrix has been derived by considering the scattering radius is known with an uncertainty $u_{R'} = 0$. The uncertainties in the third column are relative uncertainties in percentage.

4. VALIDATION

The evaluated files have been processed with the latest updates of NJOY.99 to test their format and application consistency as well as to produce a continuous-energy data library in ACE format for use in Monte Carlo codes. The ACE files have been utilized to compare results of Monte Carlo simulations using the MCNP-5 code [32] against results of measurements with a lead slowing-down spectrometer carried out by Perrot et al. [33]. In Fig. 5 the results by Perrot et al. [33] are compared with the calculated response using the evaluation presented in this report and the ENDF/B-VII.1 library. Results are shown for three different target thicknesses. This figure reveals that for both files systematic differences are observed. However, a better agreement is obtained when using the cross section file recommended in this work. This tendency becomes more obvious with increasing target thickness. The better agreement is partly due to including the parameterization in terms of average resonance parameters from 4 keV to 100 keV, which accounts for the resonance cross section fluctuations and self-shielding. However, large discrepancies remain between 1 keV and 4 keV even with the new evaluation. The differences become smaller if the upper limit of the RRR is reduced to 2 keV (instead of the original 4 keV), thus extending the URR from 2 keV to 100 keV. However, to get a full understanding of the differences a more extensive study, involving a better model of the lead slowing-down spectrometer, is required.

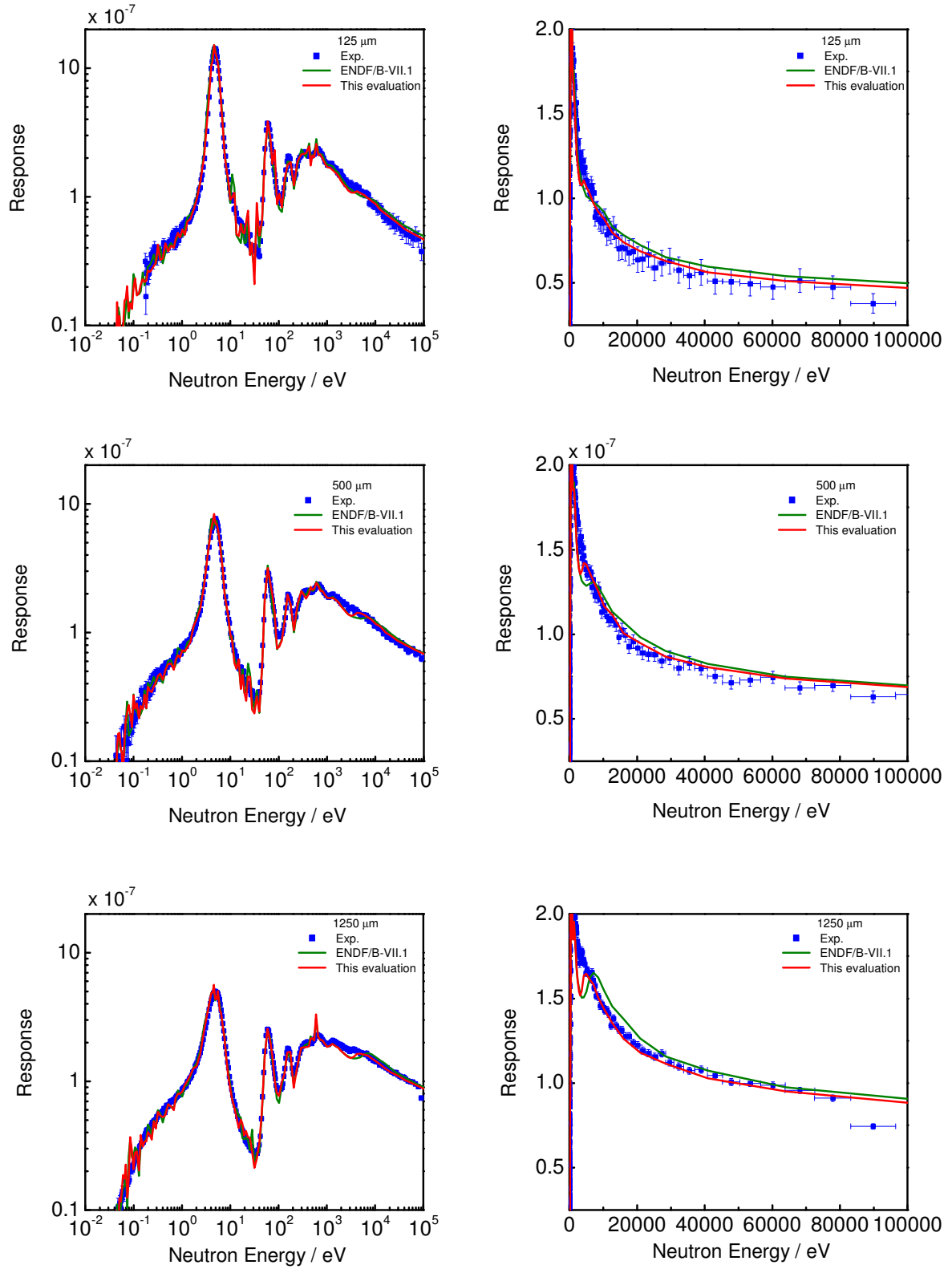


Fig. 5. Response of measurements with a lead slowing-down spectrometer resulting from prompt γ -ray measurements on Au samples of different thicknesses reported by Perrot et al. [33]. The experimental response is compared with the one calculated with MCNP using the ENDF/B-VII.1 library as well as the evaluation presented in this work.

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Title: Evaluation of neutron induced reaction cross sections on gold

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Abstract

A new evaluation of neutron induced reactions on ^{197}Au nucleus in the energy regions below 500 eV and from 4 keV to 100 keV is presented. Complete evaluated data files in ENDF-6 format have been produced by joining the evaluation with corresponding files from the ENDF/B-VII.1 library. The evaluation in the unresolved resonance region between 4 keV and 100 keV is based on a generalized single-level representation compatible with the energy-dependent option of the ENDF-6 format. The average partial cross sections have been expressed in terms of transmission coefficients by applying the Hauser-Feshbach statistical reaction theory including width fluctuations. The transmission coefficients have been obtained from a combined analysis of the capture cross section resulting from the cross section standards evaluation project and theoretical non-fluctuating cross sections derived from a dispersive coupled channel optical model. The evaluated cross sections have been validated by a comparison with transmission and capture data obtained at the time-of-flight facility GELINA. The evaluated files have been processed with the latest updates of NJOY.99 to test their format and application consistency as well as to produce a continuous-energy data library in ACE format for use in Monte Carlo codes. The ACE files have been utilized to study the effect of the evaluated resonance parameters on results of lead slowing-down experiments. The evaluated files will be implemented in the next release of the JEFF-3 library which is maintained by the Nuclear Energy Agency of the OECD.

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